

## Abstract

This invention provides an improved computationally derived regression-based method for determining  $IC_{50}$  or  $EC_{50}$  values for chemical compounds, which predicts potential drug-drug interactions involving cytochrome P450 and other enzymes, transporters, receptors or proteins with active site(s). In addition, this approach predicts affinity for target enzymes, transporters and receptor proteins from a single compound concentration, which will rapidly enable identification of therapeutic use.

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